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Socio-technical-economic assessment of power-to-X: Potentials and limitations for an integration into the German energy system

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ABSTRACT

The German Energiewende is facing new challenges with increasing shares of fluctuating renewable energies. Slow electricity grid extensions, restrictions in public perception as well as limited transformation progress in other sectors beside electricity cause major drawbacks in greenhouse gas mitigation. Power-to-X (PtX) technologies may be the missing link for a more resilient energy transition and provide both, renewable substitutes for fossil fuels as well as electricity grid balancing services owing to flexible operation and long-term storage abilities. Different PtX concepts proved operability in several worldwide distributed pilot projects. However, little is known yet about potential technical, monetary, societal and resource related scale-up limitations. In this paper, implications of these aspects for a large-scale energy system implementation are shown. From a technical perspective the concept of long-term flexible PtX operation modes is generally feasible and could become key for a more resilient future energy supply. However, economics are still the bottleneck for an extensive diffusion: in two scenarios for 2050 PtX may cause additional national annual energy costs between approx. 10 and 100 billion euros compared to an ongoing fossil fuel supply at current price conditions. Nevertheless, such expenses can be considered as reasonable in contrast to expenses for the compensation of climate change consequences of a future fossil fuel-based energy system.

1. Introduction

The energy transition in general and Germany's Energiewende in particular is based on an increasing contribution of renewable energy such as wind and solar power. Besides limited bio energy potentials, renewable electricity will be the only renewable energy source which may be utilized in all energy sectors [1]. As photovoltaic and wind power have the largest generation potential, but are highly fluctuating, there will be an increasing demand of energy storage in the long run [2]. Furthermore, to fulfill the international climate target of the Paris agreement (COP21), a limitation of global warming well below 2 °C above pre-industrial levels, greenhouse gas mitigation has to be achieved in other energy intensive sectors beside electricity as well. The electrification approach has limits, however: the globally growing aviation business as well as shipping and heavy road transport can hardly be electrified due to low volumetric energy densities of batteries [3,4]. Furthermore, industrial processes will continuously depend on hydrogen and hydrocarbon based raw materials.

Power-to-X (PtX) concepts, i.e. the conversion of renewable electricity into gases, fuels and chemicals, are considered as a major component in future energy systems [5,6]. For longer term storage, high volumetric energy density is an important issue, and this can be considered as the most prominent driving force for the development of these hydrogen based technologies [7]. All chemical PtX concepts are based on catalytic processes: Power-to-Hydrogen (PtH_2) is realized by electrolysis, i.e. electrocatalytic water splitting, which can provide hydrogen for Power-to-Methane (PtM), based on the Sabatier reaction, and Power-to-Liquid (PtL), based on either methanol synthesis or Fischer-Tropsch synthesis [8–10]. While the latter two synthesis routes are already well-established industrial processes operated at large scales, the two Power-to-Gas concepts are still subject to development and currently implemented as locally distributed applications at smaller

Abbreviations: AE, alkaline electrolysis; CAPex, capital expenditures; CCS, carbon capture and storage; FTS, Fischer-Tropsch synthesis; PEME, polymer exchange membrane electrolysis; PtH2, Power-to-Hydrogen; PtM, Power-to-Methane; PtL, Power-to-liquid; PtX, pPower-to-X; RE, renewable energy; SOE, solid oxide electrolysis; SMR, steam methane reforming; TRL, technology readiness level

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scale. Within this paper, all prior introduced PtX concepts are analyzed except Power-to-Methanol. This is due to the current debate in Germany, which focuses on electricity based synthetic hydrogen, methane and Fischer-Tropsch drop-in fuels as substitutes for conventional fuels [11].

In the course of the Energiewende, PtX utilization is motivated from different perspectives. On the one hand, fluctuations in electricity production must be balanced by dynamic conversion and storage processes to limit the necessity of expensive grid expansions, or the alternative: the curtailment of production. Having this in mind, the import of PtX products as an alternative to a national production can be relativized to some extent.

On the other hand, PtX plants of high capacities would allow for a significantly increased renewable fuel supply in all energy sectors. Hence, PtX can contribute to an advanced supply security, i.e. to a more resilient energy supply. It provides several characteristics which are assigned as *design elements* of resilient energy systems, e.g. provision of storages, buffers, diversity and redundancy [12,13]. By this means, the conversion of electricity into chemical energy will amplify the utilization of storage facilities. Furthermore, a diversification of energy resources is realized with the production of both, electricity based synthetic gases and liquid fuels. All energy carriers enable redundancies in the energy system in terms of transportation and distribution infrastructures. The fulfillment of the design elements may keep the energy system rather flexible and enable the ability to better adapt and improvise in times of unexpectable disturbing events. Thus, PtX concepts could contribute to the resilience of energy systems, enabling both, a high supply security and climate compatibility. However, PtX technologies suffer from relatively low efficiencies along the process chains. Thus, a direct utilization of hydrogen might be beneficial compared to hydrocarbon production. Nevertheless, the direct use of hydrogen, e. g. in the transportation sector, is combined with several disadvantages regarding the permeability of tanks, the ratio of volume to energy content and the necessity for a completely new infrastructure.

With the assumption of all mentioned PtX concepts being essential for a resilient energy system transformation, we evaluated potential bottlenecks and barriers for the diffusion of PtX concepts in Germany. Clustered in three sections, critical aspects were addressed from a social, a technical, and an economic perspective. Within the subsections of Chapter 2 we will focus on technical aspects such as dynamic operation potentials and scale-up limitations of small-scale demonstration approaches with low technology readiness levels (TRL) as well as raw material availability with regard to a large-scale implementation, i.e. extensive diffusion of PtX concepts. Profitability and potential acceptance issues of centralized and decentralized PtX concepts will be addressed in Chapters 3 and 4. In Chapter 5, potentials for a large-scale energy system integration of PtX and contributions to a more resilient energy transition will be discussed, followed by a conclusion in Chapter 6.

2. Assessment of required system performances and potential technical limitations

The increasing share of renewables in the German energy system requires new flexibility options. Figures from the Federal Network Agency show that *surplus energy* from renewables recently rose to a significant level with 3.74 TWh being curtailed in 2016 and 5.52 TWh in 2017 [14,15]. *Surplus energy* in this context describes energy that cannot be fed into the transmission grid due to grid congestions resulting in wind and solar generators to be shut down. Thus, this curtailed energy was actually missing in the renewable energy balance and in fact, it was not a real surplus since the electricity demand in Germany can only be covered by nearly 100% renewable energy in very rare occasions. The transmission and distribution of renewable electricity to consumers is thus a major problem in times of high production rates. With electrolyzers as controllable electricity consumers such developments could possibly be minimized if located near grid congestion hotspots. Hence, a major criteria for the implementation of PtX concepts is going to be their location.

For a large-scale fuel production, however, the utilization of fluctuating surplus energy will be considerably insufficient. Thus, besides such decentralized concepts for the electricity sector, PtX installations of high capacities will be essential for renewable fuel and base chemical production, as could be implemented e.g. at refineries. Here, a high production rate will be favorable, whereas a dynamic operation capability is of less importance. With regard to the different technical requirements for both, centralized and decentralized concepts, the two Power-to-Gas processes (PtH_2 and PtM) and the Fischer-Tropsch synthesis as an example for PtL concepts were evaluated according to three major questions:

- Is it feasible to operate catalytic PtX processes in dynamic operation for an extended period, adapted to fluctuating renewable energy supply? What impact does the dynamic operation have on life-time of PtX plants and catalyst degradation?
- Is a scale-up of PtX processes into multi-MW scale feasible in the short-to-medium term? What are potential bottlenecks?
- Is there any shortage expected in raw material supply, especially with respect to catalyst precursors? Are there limitations in CO_2 and water availability?

Within the next subsections these questions will be addressed separately to low-temperature and high-temperature electrolysis concepts as well as the Sabatier process and the Fischer-Tropsch synthesis.

2.1. Power-to-Hydrogen via water electrolysis

The expected demand of installed electrolysis power depends on the chosen scenario. For an 85% reduction of CO_2 emissions (1990 to 2050) about 5 GW of power will be required from the year 2025 on, with a steep rise up to 15 GW not before the year 2033. In 2050, however, more than 70 GW will be installed according to a prominent study by Henning and Palzer. In addition, there will be a requirement of 20 GW electrolysis power for methanation and 5 GW for production of electricity based synthetic fuels, leading to a total electrolysis power demand of nearly 100 GW. This total demand of installed electrolysis power increases up to 200 GW when considering a 90% reduction scenario instead of 85% [2]. Assumptions on electrolysis capacity demand strongly vary in a broad selection of energy transition scenarios, depending if calculations are based on more or less ambitious climate protection targets and focused energy transition pathways. In this study, however, our calculations are based on the 85% and 90% reduction scenarios of Henning and Palzer.

Plant technology for such a scenario is already available. In particular, alkaline electrolyzers are realized in multi MW scale, even though electrolysis covers only 4% of the worldwide hydrogen demand [16]. A large-scale plant, which employs conventional alkaline electrolysis, was already realized in 1970 with plant capacity of 33,000 $m^3 h^{-1}$ (H_2 atm.) [17]. This equals installed electric power of 165 MW when considering an energy demand of 5 kW h/m^3_{H2}. From this it can be concluded that the energy of a park of 80 wind mills could already be successfully converted and stored chemically.

Another factor for hydrogen production is water availability. Eight liters of water are required for the conversion of 1 kg of hydrogen in theory. In reality, especially due to losses in water purification, 15 liters of water demand can be assumed for each produced kilogram of hydrogen or 0.45 l per kWh_{H2} [18]. By this means, 450 million liters or 450,000 m^3 of water will be needed per TWh of produced hydrogen. Annual total water demand in Germany is valued at 25.1 billion m^3, whereas the potential water supply is as high as 188 billion m^3 [19]. Thus, water demand can be considered as rather uncritical.

New developments such as high temperature electrolysis (solid

oxide electrolysis, SOE), which allow for supplying part of the reaction enthalpy as heat, promise remarkable improvements of voltage efficiency (20% and above) compared to alkaline cell technology [20]. The technology profits from external input of heat that might be provided by subsequent exothermal processes (e.g. Sabatier or Fischer-Tropsch) leading to a high degree of heat integration. Its limitation, however, is the relatively low temperature level of both Sabatier and Fischer-Tropsch reactions. Further, due to the need of high operation temperature, this concept might come up with a sealing problem and severe material degradation; especially long-term stability of insulation and joining material is an issue [21]. Nevertheless, SOE is currently the most promising concept in terms of energy efficiency if heat integration is possible.

There is an ongoing debate on the risks and need of high-pressure operation of polymer electrolyte membrane electrolysis (PEME). Advantages are the possible absence of a hydrogen compressor as well as a reduction of energy consumption for compression and a reduction of overvoltage. Disadvantages, on the contrary, are a reduction of current efficiency, an increase of equilibrium potential difference, reduced life time of stack components due to hydrogen corrosion, higher investment costs and electrolyzer safety problems [22–24]. Being operated without high pressure, this technology is considered to be safe due to high product purity. When being operated at high pressure, however, there is a risk of getting mixed product gases even beyond explosive limits ("oxyhydrogen"). In order to stay clearly below the lower explosive limit, the challenge is to keep both product streams, hydrogen and oxygen, separate. The mixing risk depends on the level of the selectivity and permeability trade-off. The higher the selectivity for ion electromigration, the lower the undesired gas permeation becomes. This is, on the other hand, for the cost of relatively low ion permeability and, hence, higher internal resistance. For alkaline electrolysis (AE), which uses a diaphragm with a certain permeability for the gaseous products, the mixing risk is even more pronounced. Hence small and medium applications of these two concepts are unlikely. For more widespread applications and especially for household use, eliminating the mixing risk is of severe importance. There have been new concepts suggested for more efficiently decoupling of both half-cell reactions [25].

Thermodynamically water and the products of water splitting, oxygen and hydrogen, are in equilibrium at a voltage of 1.23 V. Water splitting electrolyzers, however, require higher voltages for the reaction to proceed in order to overcome energetic losses. This overvoltage, i.e. the part of the voltage that exceeds 1.23 V, can be divided into anodic and cathodic overpotential, which both increase with process intensity (current density) and activation energy and, thus, decrease with effectivity of the electrocatalyst used. For both part reactions, platinum alloys are currently best performers. Hence, the availability of sufficient amounts of platinum alloys could be a bottleneck [26]. While platinum is the catalyst of choice for the cathodes, it is ruthenium (and also iridium oxide) that can outperform platinum at anodes. With a demand of about 0.5 mg cm^{-2} at a cathode of polymer membrane based electrolyzers [24], this gives, when considering a power density of 5 W cm^{-2} [27], a total demand of 10 t[1] for the “100 GW power scenario”. Such an amount equals 4.6% of the global platinum use that totaled 218 t in 2015 [28]. Projected demand estimates for platinum in 2050, which did not consider the platinum demand of water electrolysis, range from 400 to 1200 t per year [29]. In comparison the global reserve (that part of the resources with a reasonable potential for becoming economically available resources) is estimated at 69,000 tons of platinum-group metals [30]. This emphasizes the need for high research efforts to replace platinum alloys by inexpensive and abundant elements such as nickel and iron.

With respect to the fluctuation of renewable energies, surprisingly little is reported in literature about the sensitivity of water electrolysis on unstable electric power supply conditions. This is an issue of highest importance as renewable energies such as wind and solar naturally fluctuate. It is known that PEME can be operated in the total partial-load range, whereas AE is limited to 20–100 % of its nominal load [22]. Furthermore, high pressure operation conditions (more than 10 bar) cause a deterioration of partial load behavior [31]. Anyhow, a more profound analysis of long term behavior under flexible load cycles has to be part of future research activities. A nickel based catalyst, for instance, as it is used in conventional anodes for alkaline water electrolysis, is stable in steady electrolysis, but it corrodes easily with potential cycling [32]. Further energy demand may rise under fluctuating conditions [33]. Another issue related to dynamic electric power supply is fluctuating temperatures within the catalytic layer causing thermo-mechanical stress. This can damage or even destroy the catalyst and is known - for catalytically coated supports - as a reason for short life times [34].

Table 1 provides an overview of relevant criteria’s for three discussed types of electrolyzers. It can be concluded, that plant technology is generally available for an extensive implementation into energy systems. However, each technology exhibits at least one constraint and that is a limited potential for dynamic operation control for AE and SOE. For PEME platinum group metals are required, which can be considered as critical resources and especially may face high expenses if the worldwide demand considerably increases.

2.2. Power-to-Methane via Sabatier reaction

The Sabatier reaction produces methane that can be considered as "*green SNG*" when "green hydrogen" and a sustainable carbon source is being used. Even though *green SNG* cannot be as cost efficient as hydrogen, it shows lower self-discharge in long term storage. The required carbon dioxide can be obtained by carbon capture from flue gas of fossil-fired power plants, e.g. via absorption (carbon scrubbing) for the cost of a high energy penalty of at least 16.3% of additional energy input [35,80]. However, the utilization of fossil-based CO_2 for electricity based synthetic fuel production enables a recycling, but does not prevent greenhouse gas emissions as long as the fuel is finally combusted again. Instead, pure CO_2 is available from biomass combustion, biogas upgrading and biofuel production with concentrations of 3–8 vol.-%, 40 vol.-% and up to 100 vol.-% respectively [35,78,79]. According to a recent study about 17 million tons of biogenic CO_2 could annually be available in Germany. This number refers to large-scaled sources (biogas-upgrading and solid biomass CHP plants larger than 1 MW_{el}) with a reasonable exploitation potential [36].

The actual CO_2 demand for PtX processes depends on the chosen scenario. Klaus et al. calculated 55 TW h of yearly methane demand until 2050. Based on the molecular weights of CO_2 and methane and related to the energy content of methane, 0.2 tons of CO_2 are required to produce 1 MW h of methane. Thus, the demand for 55 TW h will be 11 million tons of CO_2 [37]. However, biogenic CO_2 will very unlikely cover the entire carbon demand for the total electricity based synthetic fuel production due to limited sustainability potentials.

Without sufficiently high amounts of biomass, carbon dioxide needs to be recovered from air. Any kind of process requires, due to the low concentration of CO_2 in air, a throughput of 3 million cubic meters of air per ton of CO_2 recovered and even much higher amounts of energy compared to carbon capture from flue gas [38]. According to LBST, 1 ton of CO_2 from air requires 1.9 MWh_{el}, if absorption/electrodialysis technology is applied [36]. Another air capture technology was invented by the ETH Zurich spinoff Climeworks. The technology is based on an adsorption/desorption cycle, which allows to supply the major energy share in terms of low temperature heat (95 °C). The actual energy demand corresponds to 1.5–2.0 MWh_{th} and 0.2-0.3 MWh_{el}.

[1] 0.1 mg/W = 0.1 t/GW

Table 1
Overview of major criteria's for the evaluation of integration potentials for electrolyzers into energy systems. The three types are compared with concern to state of the art, scaling potentials, resources and their potential for flexible operation modes for grid balancing services [27,84,98].

Criteria	Alkaline Electrolysis	Protone Exchange Membrane Electrolysis	Solid Oxide Elektrolysis
State of the art	– Technology readiness level (TRL): 9 – Industrial application, e.g. Assuan – Capacity: 33,000 Nm^3 H_2 → 165 MW (assumption: 5 kWh m^{-3})	– TRL: 8 – Pilot projects in multi MW scale – e.g. Energiepark Mainz, 6 MW	– TRL: 5-6 – Pilot projects in multi kW scale – e.g. Salzgitter Steelworks, 150 kW
Scaling potential	– Uncritically – Large scale operation	– Uncritically – Up-Scaling in progress	– Uncritically – 20 MW plant expected in 2020
Resources	– Uncritically – Nickel catalysts	– Critical: Platinum & Iridium – Platinum group metal reserves: 66,000 t → Assumption for 10 GW: 1 t Pt → 0.5 % of worldwide demand in 2014	– Uncritically – Nickel and Ceramics catalysts
Potential for dynamic operation	– Critical – Ni-catalysts easily corrode – Load range: 20 – 100 %	– Uncritically – Catalysts remain stable – Suitable for flexible operation – Load range: < 10 – 200 %	– Critical – High thermal stresses → critical long term stability – Load range: < 50 – 100 %
Preferable application	– Preferably constant operation – Limited capability of grid balancing services – (Centralized) large scale plants	– High security – High capability of grid balancing services – (Decentralized) small to medium scale	– Suitable for sites with waste heat resources – Limited capability of grid balancing services – (Centralized) large scale plants

For an 85% reduction of CO_2 emissions (based on energy conversion) about 3 GW of installed methanation power will be required not before the year 2030. This equals 500 plants of the 6 MW type installed by Audi AG in Werlte, Germany. A steep rise, however, is expected from 2045 on, exceeding 20 GW in 2050 [2].

Today the production of „green SNG" from renewable energies in small, distributed (pilot) plants requires relatively large buffer tanks. Their volume could be reduced by dynamic production, which is technically feasible in the range of 50–100 % of a plants nominal load [39]. However changing gas loads could reduce catalyst lifetime mechanically due to thermal stress especially at the hot spot. Further a faster deactivation of the catalyst is possible. A more dynamic operation can be expected when using monolithic sponges with improved heat transport by conduction allowing for better hot spot control.

The state of the art catalyst for Sabatier reaction is nickel which provides high methane selectivity and relatively high yield. Ruthenium, however, is even more active: for a single tube reactor with a turnover rate of 1.7 kg/(m^2*s) the necessary catalyst load is 3.5 g ruthenium to convert 12 kW.[2] From this it can be estimated that, for a capacity demand of 20 GW in 2050, 5.8 tons of ruthenium will be required in total. This equals about 0.01% of the world's global reserve of platinum-group metals and nearly 45% of US ruthenium imports in 2017 [30].

When using nickel instead, its comparatively lower activity requires higher temperatures for obtaining the same reaction rate. This in turn restricts the yield of the reaction even at multi-stage operation with intermediate cooling. It is due to the thermodynamics of exothermal reactions - such as Sabatier reaction – that reactions yield decreases non-linearly with increasing temperature. Recently it was shown that cobalt, an element almost as well-available as nickel, performs much better in this respect: If particle size of cobalt coating is properly chosen, a temperature of 300 °C is sufficient for a reasonable turnover frequency [40], for which nickel requires higher temperatures. However, this needs to be confirmed at large-scale.

Assuming that the activity of nickel is one tenth of the activity of ruthenium, about 60 tons of nickel will be required to realize a methanation capacity of 20 GW. Since this is no more than 0.003% of the actual global mine production capacity per year [41], there is no limitation to be expected with respect to raw material supply for the production of Sabatier reactors.

Given a limited yield of about 85%, the Sabatier reaction provides a product with a concentration of carbon dioxide and hydrogen which is too high for many applications. Subsequent purification by state of the art treatment processes, such as absorption, adsorption or membrane separation is expensive and reduces the overall process energy efficiency. Therefore, all efforts in further process development should aim at improved highly-performing, low-cost catalysts to allow for highest yield conversions. The higher the activity, the shorter the reactor length required for that high yield. Thus, depending on the activity, capital expenses of the methanation process will be determined either by the price of steel (on top of engineering and instrumentation cost) at lower activity or by peripheral equipment and engineering alone.

2.3. Power-to-Liquid via Fischer-Tropsch synthesis

Fischer-Tropsch synthesis (FTS) is a much more complex reaction compared to Sabatier reaction as it converts carbon monoxide and hydrogen into a mixture of gaseous and liquid hydrocarbons. This complexity is one reason for the current preference to operate FTS stationary at large-scale only. It is a process that has been applied for decades in coal liquefaction with production rates of low-sulfur diesel fuel in the order of magnitude of 1 million metric tons per year. First attempts for scaling down FTS-plants turned out to be challenging. Nevertheless, with the high heat removal capability of microreactor technology, single pass conversions of up to 75% have been realized [42]. Higher conversions are challenging as they lead to high concentrations of water that can result in reoxidation of the active cobalt catalyst.

Like Sabatier reaction, FTS is a strongly exothermal process requiring permanent cooling to prevent hot spots or even run-aways. In case of FTS cost and temperature is even more important, as the product composition is very sensitive on temperature changes. While Sabatier reaction produces methane only, the product in FTS comprises alkanes, alkenes, alcohols, and other oxygenated hydrocarbons. The increased process complexity causes a slower partial load behavior than known from the Sabatier reaction. However, dynamic partial load operation can be realized with a minimum of 50% of the nominal load and is therefore still in a feasible order of magnitude [39]. Subsequent to FTS, the product mixture is to be refined, similar to crude oil. Any changes in composition would increase downstream processing demand. All this makes dynamically operated small-scale plants challenging.

Expected power demand will be, according to the 85% CO_2-reduction scenario, about 2 GW, 4 GW and 5 GW in the years 2022, 2027, and 2030 respectively [2]. This demand can be considered in context with the performance of a large-scale production facility for transforming syngas into liquid, e.g. Pearl, Qatar [43]. Substitution of its production capacity (140,000 BPD) by means of electricity based FTS fuels would

[2] Case study (p0 = 10 bar, T0 = 300 °C, Da = 0.1, Se = 2.55, Y = 92%, L = 0.5 m, D = 25 mm) according to Kiewidt and Thöming [83]

Table 2
Overview on major criteria's for the production of hydrocarbons via PtG and PtL. Both discussed processes are compared regarding state of the art, scaling potentials, resources and their potential for flexible operation modes for grid balancing services [84,98].

Criteria	Sabatier Process	Fischer-Tropsch Synthesis
State of the art	– TRL: 6-8 – Pilot projects in multi MW scale – e.g. Werlte, 6 MW	– TRL: 9 – Industrial application – e.g. syngas to liquid in Pearl, 140,000 BPD → 170 MW
Scaling potential	– Uncritically	– Down scaling rather critical
Resources	– Uncritically: Nickel catalysts as standard – Alternatively Ruthenium – Perspectively Cobalt	– Uncritically: Iron and Cobalt – Alternatively Ruthenium
Potential for dynamic operation	– Critical – Thermal stress at inconstant gas production → Limited catalyst lifetime → More active catalyst or buffer storage required	– Critical – Highly exothermal process → Constant cooling required → Hazard: Hotspots & thermal runaway → Optimized heat management for high product quality required
Preferable application	– Generally (decentralized) dynamic and (centralized) constant operation modes possible	– Centralized large scale plants at constant operation mode

cause a power demand of about 18 GW,[3] which is already more than three times the predicted demand for 2030. CO_2 demand for the PtL process depends on the chain lenghts of produced hydrocarbons. Recent studies suggest 0.27-0.34 tons of CO_2 for 1 MW h of electricity based synthetic crude oil substitute [9,44]. In an extreme case scenario for a greenhouse gas neutral energy supply in Germany, 552 TW h of electricity based synthetic liquid fuels are projected for 2050, involving a CO_2 demand of 149–187.7 tons [45].

Currently the catalyst's elements, which are usually considered as most relevant for future applications, are Fe, Co, and Ru. While the latter two remain in the metallic state under the reducing conditions during operation, iron catalysts form a number of oxides and carbides during reaction. This necessitates control of these phase transformations in order to maintain catalytic activity. Availability of catalyst is not a limiting factor. For 5 GW the total mass of catalyst required is 200 t of active element.[4] In case of iron, the fourth most abundant element in Earth's crust, this amount is negligible. The same with cobalt (refined cobalt production 2015: 97,400 t per year) [46]. Ruthenium, on the other hand, is much too expensive to be used as main active component. However, even as minor component of about 1 wt.-% the amount required is still in the order of magnitude of 2 t, which is quite a lot when considering that the global consumption of ruthenium was 34.2 t in 2016 [47].

The active catalyst is obtained on stream. Iron, the most prominent Fischer-Tropsch catalyst, is not active by itself, even when being in the reduced state. It is rather an iron carbon compound which requires days or even weeks to be formed during operation. Thus, it takes a certain period of time to reach reasonable yield and selectivity. The other candidate is cobalt, which produces methane when carbon dioxide is used as feed and becomes highly Fischer-Tropsch active when carbon monoxide is used instead. Like iron, cobalt has to be reduced at hydrogen atmosphere before usage.

Both catalysts are based on abundant raw materials and can be produced by relatively simple precipitation processes. Recently it was found, however, that more sophisticated coating processes, such as sol-gel techniques, allowed for control thickness of catalyst layer as well as size of cobalt nanoparticles. By this means, the best compromise for reducibility and activity can be achieved [40].

In contrary to the raw materials of the catalysts, which are relatively cheap (in case of cobalt about 65,000 €/t) [48], steel required for piping and reactor tubes and vessels determines the plant cost. However, this has to be qualified since the cobalt price increased by 113% from 2016 to 2017 [48]. This is, inter alia, due to the rising demand for lithium-ion battery cathodes [49]. A continuation of this development might refute the initial statement.

Table 2 comprises the major technical evaluation results for both discussed hydrocarbon generation processes, Sabatier process and Fischer-Tropsch synthesis. For both processes it can be concluded that a dynamic operation control remains critical as long as catalysts with comparably low activity are applied. By this means hydrogen buffer tanks for constant process operation would be needed. However, there are research efforts for a small scale flexible process design of Fischer-Tropsch reactors [50].

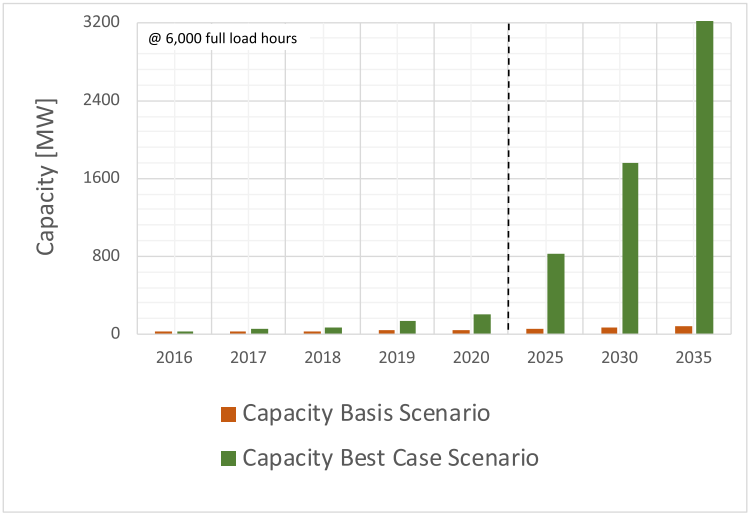
3. Economic evaluation of centralized and decentralized PtX concepts

The results of the previous subsections show that both, large-scale (centralized) and small-scale (decentralized) concepts are generally realizable from a technical perspective. This sections focus is on the economic viability of such PtX approaches. The most prominent economic dilemma is given by the contradiction of a maximized PtX plants annual operation time and the provision of system services to minimize the curtailment of renewable energy. For a reduction of wind power down throttling, excess PtX capacity is required.

Repeatedly it is argued that a further improvement of voltage efficiency of the electrolysis could solve the economic problem. However, in a recent study it was shown that business cases can hardly occur even at high utilization rates of 6000 full load hours for centralized concepts and progressively assumed technical improvement. An agent-based model was developed to investigate business case evolvement and related capacity growth depending on several adjusted framing conditions. Based on stakeholder information, representative investor and customer groups for PtX were characterized and implemented as agents, which aim to sell and buy PtX products in the national energy markets. Related to their individual characteristics, the agents attempt to create business cases and/or purchase PtX products at specific price thresholds. Based on the development of demand and business cases in a defined time horizon, the resulting capacity growth could be

[3] Assumption: 1 barrel = 1,700 kWh; Conversion Efficiency:η = 55 %

[4] Given a typical space velocity of 0.1 mol synthesis gas per kg catalyst per second (catalyst: active elements, without weight of alumina support) Estimation: heat of combustion CH_4 = 880 kJ/mol and 0.03 mol CH_4/(kg s) gives 26 kJ/(kg s) = 26 kW/kg catalyst, which equals 80 t



Net market prices in Germany (2016)

Electricity:	2-3 ct kWh^{-1}
Gas:	1-3 ct kWh^{-1}
Petrol/Diesel:	4-7 ct kWh^{-1}
Biofuels:	7-8 ct kWh^{-1}
Hydrogen (SMR):	6-7 ct kWh^{-1}

	2035	
	CAPex [€ kW^{-1}]	Product [ct kWh^{-1}]
$P2H_2$	1,292	23.6
P2M	2,630	30.4
P2L	3,500	38.7

	2035	
	CAPex [€ kW^{-1}]	Product [ct kWh^{-1}]
$P2H_2$	520	12.8
P2M	1,000	15.4
P2L	1,000	15.4

Fig. 1. Simulation results for PtX capacity growth until 2035 and related production costs for hydrogen as well as electricity based synthetic methane and liquid fuels in two scenarios: In a *Basis Scenario* todays legal framing conditions remained unchanged throughout the model run. In a *Best Case Scenario*, framing conditions were optimized and allowed reduced production costs and capital costs as a result of scaling effects [51].

evaluated. With the adjustment of framing conditions in specific scenarios, the most important parameters for a successful diffusion of PtX were characterized. It was revealed that a high diffusion of electricity based synthetic fuel production rather requires consequent research funding and subsidies for the construction of new installations to enable capital expenditures (CAPex) reduction through scaling effects. Furthermore, strict greenhouse gas mitigation quotas for industries need to be implemented to achieve competitiveness to fossil fuels. In a best case scenario without surcharges for input electricity, production costs of 12.8 cent kWh^{-1} for hydrogen and above 15 cent kWh^{-1} for methane and liquid fuels were calculated [51], also see Fig. 1.

In addition, Henning and Palzer showed that for a total conversion of the energy system and for a nearly full wind energy usage (almost no down throttling), the demand of electrolysis plants will be about 100 GW of installed electric power. This in turn leads to operation times as low as 2,000 h per year and costs of about 18 ct kWh^{-1} of hydrogen. With reduction of installed power below 20 GW, however, the operation times improve slightly progressively, while the improvement of cost is disproportionally lower: For exceeding an operation time of 5,000 h per year the cost drop down to 13 ct kWh^{-1}H_2 only [2]. Table 3 comprises typical net price ranges for fossil fuels, electricity and hydrogen from steam methane reforming (SMR). At current legislation, input electricity for PtX processes is surcharged with high additional fees and taxes, if product X is not used for electricity generation.

Profitability is mainly dependent on investment costs, costs for input electricity, number of full load hours and revenues at appropriate markets. Whereas even centralized concepts with high utilization rates can hardly run economically, business cases might be even harder to create for decentralized PtX concepts with a low utilization in times of high electricity production only. Therefore, two different cases for decentralized concepts are compared:

- A PtX entity is directly connected to a renewable energy unit and converts surplus electricity into electricity based synthetic fuels.
- A PtX entity is directly connected to a renewable energy unit which was constructed for electricity based synthetic fuel production only and is not connected to the power grid.

In both cases the PtX entity may not be in the duty of compensating any fees for input electricity as it is disconnected to the public electricity grid. For the first case, the intended benefit for the energy system could be a reduced demand for power grid extensions. As grid extensions are expensive and much slower than RE expansion (e.g. due to lack of social acceptance, [52]), such a concept would be highly attractive: Surplus energy will be chemically stored and used in other sectors or reconverted to electricity in times of low wind and photovoltaic power. The above mentioned increasing curtailment of renewable electricity, which caused a financial damage of 610 million euros in 2017 and is leading to increasing network fees for consumers, might be balanced [15].

Table 3
Overview of fossil fuel net prices and hydrogen from steam methane reforming [87,90]; [93,96]. Input electricity for PtX processes is further surcharged by fees and taxes at current legislation in Germany [86,89]. Assumptions on investment costs are based on [92,21,85,91,94,95,97].

Energy carrier	Prices		Technology	CAPex
	€ kWh^{-1}	specified units		€ kW^{-1}
Natural gas	0.01-0.03	0.08-0.25 € Nm^{-3}	*Alkaline electrolysis*	800-1,500
Crude oil	0.05-0.07	85-119 € bbl^{-1}		
			Protone exchange membrane electrolysis	2,000-6,000
Bio fuels				
Gas	0.08	0.88 € Nm^{-3}	*Solid oxide electrolysis*	2,500-8,000
Diesel	0.08	0.83 € l^{-1}		
Petrol	0.07	0.68 € l^{-1}	*Methanation*	720
Hydrogen	0.06	0.21 € Nm^{-3}	*Fischer-Tropsch Synthesis*	1,000
Electricity	0.02-0.03			
- Surcharges for PtX entities in 2016	0.196			

The German Energy Agency expects limited feed-in of 80% for wind and 70% for photovoltaic installations of their theoretical peak power, since costs for power grid extensions would increase inversely proportional related to the additional energy yield [53]. Brunner et al. calculated resulting full load hours for the first case based on load profiles and the assumption of 4000 utilization hours of photovoltaic and 7000 utilization hours of onshore wind power and the reduced feed-in of 70% and 80% of the theoretical peak power. In accord, photovoltaic power would be curtailed 83 h per year and onshore wind power for 46 h per year. From this it was presumed that a resulting full load operation of below 100 h will eliminate profitability even at free input electricity and CO_2 because of too high CAPex. But even progressive investment cost reductions will not help to create business cases at low utilization rates. For hydrogen production costs of 1.76–6.11 € kWh_{H2}^{-1} were calculated, which is up to factor 100 higher than hydrogen from SMR according to Table 1 [54]. However, as stated in Chapter 2, dynamic PtX concepts require additional expenditures which were not considered in this calculation. Thus, the barrier for profitability will further increase. Electricity based synthetic methane production would end up even more expensive due to lower process efficiency and higher CAPex. The Fischer-Tropsch synthesis instead is not applicable for such low operating hours due to complex process control.

In the second case it is assumed that the renewable energy source was installed to serve PtX entities only. Thus, electricity costs need to be calculated as high as the production costs of the renewable source according to plant life-time. A direct connection to PtX plants exhibits several advantages. As the public power grid is not used, corresponding charges, fees and taxes do not need to be compensated. In accord to resilience such concepts are beneficial as well, since fuel and base chemical production becomes at least partly independent from power networks and possible shortages. In this case it requires optimized scaling of input power of the PtX installation and output power of the renewable energy source to grant high utilization rates. Thus, the PtX installation capacity should be significantly lower than the capacity of the RE plant.

Kost et al. calculated RE production costs of 4.5–10.9 ct kWh^{-1} for wind onshore and 8.0–14.0 ct kWh^{-1} for photovoltaic electricity, individually dependent on utilization and location. Future developments are estimated to range between 4.2–10.2 ct kWh^{-1} and 5.5–9.5 ct kWh^{-1} [55]. With regard to these assumptions it can be expected that business cases may arise, if CAPex degression for both, RE and PtX plants occur, combined with high utilization rates as well as increasing prices for fossil energy. However, high utilization rates require dynamic operation capability, leading to more extensive investment costs compared to power grid connected concepts.

4. Evaluation of potential limitations in social acceptance

The existing pilot projects in Germany did not experience problems concerning social acceptance [56]. Furthermore, direct utilization of hydrogen did not appear to be confronted with safety issues [57]. Instead of potential scandalization and limited acceptance, a few of these projects rather achieved support by a better willingness to pay of customers for the electricity based synthetic products. The motivation to support the development of PtX innovation is seen as a main driver for the higher willingness to pay. As stated above, the PtX concept is widely recognized as a future core element of the energy system transformation process. It allows for a shift of renewable electricity to other sectors and this way enables a “green” gas und fuel consumption for the first time without the use of biomass. In accord, it may be expected that especially decentralized small-scale PtX concepts for the utilization of excess electricity will not be confronted with scandalizing processes. Instead, communities aiming for a self-sustaining energy supply are aware that PtX may become a major component within local energy systems [12].

In general it is acknowledged that energy storage and conversion concepts are better accepted than infrastructural measures such as power grid extensions [31]. The latter is one of the major drawbacks in the German energy transition as nearby installations are often refused by activists. However, a consequence of slowed grid extensions are increasing curtailed excess electricity volumes. The compensations for RE plant operators in turn increase electricity prices, leading to new constraints for the Energiewende. Thus, energy storage and conversion concepts such as PtX may be the missing link to solve both, perception problems as well as lacked excess electricity utilization. Buenger et al. report that energy providers see PtX installations to compensate for bottlenecks in transmission networks. However, PtX may rather complement and not compensate grid extensions [58].

Experience with centralized large-scale PtX entities is not available. A look at previous technological innovation processes reveals that especially research and pilot projects are often better perceived than first attempts of large-scale implementations, e.g. in case of CCS (carbon capture and storage) projects [59]. CCS was formerly seen as a major innovation for reaching the greenhouse gas emission targets in many German economic optimization models. In consequence of serious scandalizing processes in public, however, CCS projects were barely ever realized in Germany [60].

However, such cohenrences are strongly dependent on situational factors. Sonnberger et al. recently stated impact factors having an effect on social acceptance for energy technologies. They found four key values determining acceptance: confidence in companies and/or actors, general attitude to the Energiewende, perceived fairness of the Energiewende, perceived benefit of the technology and perceived risks and disadvantages of the technology. Thus, citizens are willing to support transformation processes if they are convinced of the purpose. If this is the case people most likely will be willing to contribute [61].

The promotive support of well trusted research institutes as well as of prominent NGO’s may also indicate a high acceptance potential for PtX installations beyond pilot scales. Nevertheless, even though large-scale installations may not experience acceptance issues directly, the increasing demand for renewable electricity for electricity based synthetic fuel production may lead to indirect scandalizing processes. Depending on the chosen scenarios, a coverage of the total national fuel and base chemical demand may lead to increasing renewable energy capacities up to factor 15 compared to today’s share [45,62,63]. This is also because of high conversion losses which might further decrease acceptance for PtX processes. Today, critics of renewable energy, especially of wind power, argue with spoiled landscapes, hazards for endemic bird populations and harmful noise pollution. Another major argument is that, even though visible to a large extent, renewables contributed to a share of only 15% of the end energy consumption in 2015 [64]. So the source of expectable main objections against the development of PtX will not be in the conversion technologies themselves but in the enormous extension of wind energy, especially onshore.

However, according to recent surveys, 93% of the German population believe that the expansion of renewables is of exceptional importance. 62% stated to support new installations in their surrounding neighborhood. Thus, the “not in my backyard” phenomenon may only affect the extension of onshore wind energy plants. At least, a higher support of residents living close to renewable energy installations compared to others appears to be present [65,66].

With regard to the PtX concept an overall conclusion whether acceptance will remain high or decrease during an extensive energy system integration process is not possible. However, with a focus on the whole transformation process PtX may technically solve current critiques such as lacked excess electricity utilization and this way increase its perception. Nevertheless, a national and completely renewable fuel supply from German production will be very unlikely, limiting the national PtX capacities as well. Thus, the Federal Environment Agency suggests to import electricity based synthetic fuels to a large extent directly from abroad, where larger area potentials are available [67]. As

Table 4
Comparison of the demand for electricity, gas and liquid fuels and available storage capacities [88].

		Electricity	Gas	Liquid fuels
Demand	[TWh a^{-1}]	610	909	711
Average power	[GW]	70	100	80
Storage capacity	[TWh]	0,04	217	250
Share of renewable energies	%	˜ 36	˜ 1.5	˜ 6

already mentioned in the introduction this serves well for uncritical infrastructures and other services. However, from a resilience point of view a large scale national PtX diffusion would be favorable and could be supplemented by imports.

5. Contributions and restrictions to a resilient energy system transition

As stated above, an extensive implementation of PtX is beneficial in order to implement some design elements into energy systems. According to Table 4, there are large capacities for gas and liquid fuel storage available in Germany, whereas only a low capacity of pumped hydro storage for electricity generation is available. With PtX, the large storage capacities for methane and liquid fuels can remain sustained and contribute to a less vulnerable future energy supply.

Table 4 also indicates a comparably low share of renewables in gas and liquid fuel supply, i.e. in the heat, industry and mobility sectors. Nevertheless, as stated above, hydrocarbon-based fuels will also play a significant role in a future CO_2 neutral energy system. Today, this small share is provided via biofuels. However, due to land use conflicts, fuels generated via PtX are widely recognized as an advantageous alternative [68,69].

Within the previous sections it was revealed that PtX concepts are technically feasible, even for flexible operation modes and excess electricity utilization and thus have a high potential to contribute to a more resilient energy transition. However, several limiting factors, especially economic feasibility, may restrain the diffusion of PtX. In Section 3 it was pointed out that, even in a *best case scenario*, electricity based synthetic fuels will not be competitive to today's fuel prices. Thus, the substitution of fossil fuels may induce a much more expensive future fuel supply of above 12 ct kWh^{-1} for hydrogen and more than 15 ct kWh^{-1} for methane and liquid fuels, even if legal framing conditions are widely adjusted. This, however, may arouse societal problems and requires further consideration.

According to a prominent study from the Federal Environment Agency, the national fossil fuel consumption in all sectors was 895 TWh of natural gas and 696 TWh of liquid fuels in 2010 [70]. Based on the prospected electricity based synthetic fuel demand for 2050 in an extreme case scenario for a greenhouse gas neutral energy system [70] and calculations in Table 5, the annual national expenses for a renewable gas and liquid fuel supply via PtX could almost treble with up to 175.4 billion euros compared to 59.6 billion euros for fossil fuel supply at constant price conditions. However, in a more moderate scenario for a 85% greenhouse gas reduction until 2050 compared to 1990 from Henning and Palzer, the assigned PtX demand is considerably lower with only 29.4 TWh of methane and 27.3 TWh of liquid fuels [2]. Based on the production costs from Fig. 1, the annual costs for electricity based synthetic methane and liquid fuels would sum up to 8.7 billion euros in this scenario, respectively. Thus, the additional expenses for PtX are not only related to chosen technical transition pathways but also to the greenhouse gas reduction goals.

Nevertheless, according to a study from the German Institute for Economic Research, the expenses for the compensation of climate change consequences could sum up to 800 billion euros until 2050 and 3000 billion euros until 2100, if any further climate protection measures are applied [71]. This indicates that resilience efforts like a PtX implementation can still be considered generally economically worthwhile on the long scale, even though such a system will be much more expensive than the fossil-based system of today. The assumptions also correlate to findings of Burke et al. who investigated the negative impacts of global warming on the global economic output [99]. Furthermore, financial penalties for missed climate protection targets must not be neglected within this discussion. Following the current trend, Germany will not reach its climate protection targets for 2020 and 2030 and will have to financially compensate its excess emissions. According to Deutsch et al. up 60 billion euros of penalty expenses might occur for Germany until 2030 at the current trend [72].

6. Conclusion

In general, studies from well renowned research institutes see PtX as a major component in future energy systems. This is especially related to the potential provision of system services, e.g. chemical long term storage of electricity and electricity based synthetic fuel production as well as balancing fluctuating renewable energy supply. Alternatively, an "all electric" world is not a reasonable scenario and, as stated in Chapter 4, CCS technologies are not considered sustainable and face serious acceptance problems. However, most of the studies do not consider possible limitations of PtX concepts to fulfill the requirements. In terms of a resilient energy system transition, we focused on potential technical, monetary, societal and resource related scale-up limitations.

Within the previous sections it was revealed that the technology of chemical energy storage with PtX processes is generally available. Even consumption of total excess electricity via PtX appears technically feasible. However, costs increase nonlinearly with avoided energy losses, and for all PtX processes high capital expenses have been calculated. This CAPex problem as well as disadvantageous legal framing conditions are considered to currently hinder applications beyond pilot scale and appear to be the most limiting factor for an extensive integration of PtX into energy systems. As an approach for CAPex

Table 5
Comparison of total expenses for the national gas and liquid fuel consumption based on fossil sources and on PtX processes. Calculations are based on mean values from Table 3 and assigned PtX production costs from Fig. 1. Consumption values for 2010 and 2050 are based on an extreme case scenario from the Federal Environment Agency [70].

	Energy source			Energy source	
Final energy consumption 2010	*Natural gas (TWh)*	*Liquid fuel (TWh)*	*Final energy consumption 2050*	*Power-to-Methane (TWh)*	*Power-to-Liquid (TWh)*
	895	696	assumed in *UBA THGND scenario*	587.7	551.9
Fossil	*Natural gas*	*Liquid fuel*	***PtX***	*Natural gas substitute*	*Liquid fuel substitute*
in €kWh^{-1}	0.02	0.06	***in € kWh^{-1}***	0.128 - 0.154	0.154
Total costs (fossil) in billion euros	17.9	41.7	***Total costs (PtX) in billion euros***	75.2 - 90.5	84.9
Sum in billion euros	59.6		***Sum in billion euros***	160.1 - 175.4	

reduction, diminishing storage volumes for hydrogen has been suggested by applying dynamic operation of the processes. On the other hand, this concept drastically enlarges the PtX processes and thereby CAPex of these processes. Furthermore, any dynamic operation requires catalysts with high thermal stability as well as excellent thermo-management to avoid temperature peaks. This includes the usage of platinum group metals, e.g. for PEME, which are considered as scarce resources. Even though reserves might not be considered as critical today, prices could dramatically increase if a worldwide demand for multi GW PtX installations arises. Thus, the availability of scarce raw materials should be further investigated and the catalysts play another key role for cost minimization. This could be possible either by replacing noble metals by more abundant and cheap elements and improving their activity. Especially the latter could allow for process intensification which results in improved space-time yields, i. e. increased throughput and smaller plants.

Another cost factor is process safety: In case of electrolysis it is the mixing risk of getting explosive hydrogen, while the other processes require expensive cooling systems. Decentralized miniplants would therefore require inherent safety concepts. Furthermore, all plants have to be gas-tight which could become a challenge at elevated temperatures. High temperature electrolysis (SOE) profits from external input of heat that might be provided by exothermal processes leading to a high degree of heat integration. In contrary to alkaline electrolysis, PEME provides hydrogen of relatively high purity. The Sabatier reaction, however, requires some purification effort because of limited yield. Depending on the application of methane, residual carbon dioxide might be removed by processes, such as membrane filtration or absorption. The highest effort is required for downstream processing of FTS product streams. In this case cracking and thermal treatment stages are needed. This is not only a fuel quality issue but also determines fuel availability. Finally, fuel availability stands or falls with physical storage capacity, i.e., size of tanks.

Nevertheless, in Chapter 5 it was discussed that high national expenses for PtX processes and the related products always need to be compared with avoided costs of climate change consequences and saved penalty costs for missed climate protection targets, respectively. Given the advantages in the context of contributions to a more resilient energy supply, the additional national energy costs might be considered as economically worthwhile.

In Chapter 3 is was pointed out that further funding for new PtX projects is required to achieve CAPex reduction through scaling effects. According to the requirement of both, flexible operation for grid balancing services as well as large-scale fuel production, we propose more financing of pilot projects as a key mechanism for PtX plant optimization and market integration. The new energy research program of the German government will allow for such new projects [73]. However, business models can hardly develop at current legal framing conditions. Thus, supportive regulations for the production and consumption of renewable electricity based synthetic fuels are also required. Fixed feed-in tariffs might also be discussed as an indirect funding mechanism. Nevertheless, even on a long scale perspective it may be unlikely that PtX products become competitive to today's fossil fuel prices. Higher EU ETS certificate prices or the introduction of carbon taxes for fossil fuels would accelerate economic competitiveness of PtX products.

On a time scale, hydrogen production via electrolysis appears to be the first application of PtX, either for direct use, e.g. hydrogen mobility or integrated in industrial processes for the replacement of SMR. An upscaling progress of electricity based synthetic hydrocarbon production via FTS or Sabatier process is rather important for further proof of concept today, since the share of renewable energy remains too low for a large-scale electricity based synthetic fuel production. However, with increasing renewable energy capacities, all PtX processes are of significant importance and can contribute to sustainably supply all energy sectors with electricity based synthetic fuels, compensate fluctuations of renewable energy supply and increase the resilience of the overall energy system.

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